HYDRATION OF AN ACID ANHYDRIDE: THE WATER COMPLEX OF ACETIC SULFURIC ANHYDRIDE

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The water complex of acetic sulfuric anhydride (ASA, CH_3COOSO_2OH) has been observed by pulsed nozzle Fourier transform microwave spectroscopy. ASA is formed in situ in the supersonic jet via the reaction of SO_3 and acetic acid and subsequently forms a complex with water during the expansion. Spectra of the parent and fully deuterated form, as well as those of the species derived from $CH_3{}^{13}COOH$, have been observed. The fitted internal rotation barrier of the methyl group is 219.599(21), cm^{-1}indicating the complexation with water lowers the internal rotation barrier of the methyl group by 9% relative to that of free ASA. The observed species is one of several isomers identified theoretically in which the water inserts into the intramolecular hydrogen bond of the ASA. Aspects of the intermolecular potential energy surface are discussed.